



KAISER ♦ HILL  
COMPANY

**Fiscal Year 2000  
Actinide Migration Evaluation  
Data Quality Objectives**

**FINAL  
Revision 6**

**April 11, 2000**

**Rocky Flats Environmental Technology Site  
Golden, Colorado 80402**

DOCUMENT CLASSIFICATION  
REVIEWED BY PER  
CLASSIFICATION OFFICE



**ADMIN RECORD**

SW-A-004167

## CONTENTS

	<b>Page</b>
<b>PURPOSE AND SCOPE</b>	<b>4</b>
<b>DATA QUALITY OBJECTIVES</b>	<b>5</b>
THE PROBLEM	5
THE IDENTIFIED DECISION	5
INPUTS TO THE DECISION	5
Urgent Data Needs for Decision Input	7
Near and Long-Term Data Needs for Decision Input	7
STUDY BOUNDARIES	13
Boundaries for Urgent Protection of Surface Water	13
Boundaries for Near-Term Protection of Surface Water	13
Boundaries for Long-Term Protection of Surface Water	13
DECISION RULE	14
LIMITS ON DECISION ERRORS	14
OPTIMIZATION OF DESIGN	14
<b>LIMITS OF MEASUREMENT UNCERTAINTY</b>	<b>14</b>
ANALYTICAL REQUIREMENTS	15
ACCURACY	15
PRECISION	16
REPRESENTATIVENESS	17
COMPARABILITY	17
COMPLETENESS	17
STATISTICAL SAMPLING/SUB-SAMPLING	18
VALIDATION	18
MODEL REQUIREMENTS	18
SENSITIVITY AND UNCERTAINTY ANALYSIS	18
CALIBRATION	20
MODEL VERIFICATION/VALIDATION	21
REFERENCES	23

### Tables

#### Table 1

Summary of Basic Actinide Transport Processes and Associated Actinide Sources and Models to be Assessed

#### Table 2

Data Needs, Availability, and Attainability for Investigation of Water-Quality Standard Exceedances

## Acronyms/Abbreviations

AME - Actinide Migration Evaluation  
ASD - Analytical Services Division  
CSM - Colorado School of Mines  
CSU - Colorado State University  
Deg - degrees  
DEM - Digital Elevation Model  
DER - Duplicate Error Ratio  
DO - Dissolved Oxygen  
DOC - Dissolved Organic Carbon  
DQO - Data Quality Objectives  
FY - Fiscal Year  
GIS - Geographical Information System  
IA - Industrial Area  
IM/IRA - Interim Measure/Interim Remedial Action  
LANL - Los Alamos National Laboratory  
LCS - Laboratory Control Standards  
M/s - meters per second  
mrem - millirem  
mg/L - milligrams/liter  
mm - millimeter  
OU - Operable Unit,  
 $\mu\text{m}$  - microns  
MDA - Minimum Detectable Activity  
NWS - National Weather Service  
PARCC - Precision, Accuracy, Representativeness, Comparability, Completeness  
pCi/g - picocuries/gram  
Pu - Plutonium  
QA/QC - Quality Assurance/Quality Control  
RFCA - Rocky Flats Cleanup Agreement  
RFETS - Rocky Flats Environmental Technology Site  
RMRS - Rocky Mountain Remediation Services LLC  
SID - South Interceptor Ditch  
SOW - Statement of Work  
SWD - Surface Water Database  
TAMU - Texas A&M University  
TOC - Total Organic Carbon  
 $\mu\text{m}$  - micrometer  
USDOE - United States Department of Energy  
USEPA - United States Environmental Protection Agency  
USGS - United States Geological Survey  
V&V - Verification and Validation

## Purpose and Scope

The purpose of this document is to outline the Data Quality Objectives (DQOs) for the Actinide Migration Evaluation (AME) group at the Rocky Flats Environmental Technology Site (Site). The AME group is being implemented to investigate the mobility of plutonium, americium, and uranium in the Site environment. The goal of the AME group is to answer the following questions in the order of urgency shown:

1. Urgent What are the important actinide migration sources and migration processes that account for surface water standard exceedances?
2. Near Term What will be the impacts of planned remedial actions on actinide migration? To what level do sources need to be cleaned up to protect surface water from exceeding action levels for actinides? To what level do emissions need to be controlled from remediation and D&D activities to be protective of air quality?
3. Long Term How will actinide migration affect surface water and/or air quality after Site closure? In other words, will soil action levels be sufficiently protective of surface water and/or air over the long term? ?
4. Long Term What is the long-term off-site actinide migration, and how will it impact downstream or downwind areas (e.g., accumulation)?

These questions will be answered by measuring and modeling actinide transport processes to understand and predict 1) actinide concentrations and total loads to surface water and 2) air concentrations and particle deposition via air transport attributed to all sources of actinides in the Site environment. The USEPA DQO process was used as a foundation for establishing the necessary quality of input data for analytical processes and the mathematical actinide mobility models (USEPA, 1994) and (USEPA, 1993). The models will be used to estimate the fate of actinides transported to surface water via each environmental pathway and evaluate the potential for air concentration exceedances. These models will be evaluated using the criteria described later in this document. This criteria have been compiled from several sources including the ASCE task force on the Criteria for Evaluation of Watershed Models (ASCE, 1993) and the CAMASE guidelines (CAMASE, 1995) for argo-ecosystems modeling.

The scope of this document is currently limited to establishing DQOs for actinide migration research for the pathways listed below. Additionally, the results of the pathway analyses may be used to support the comprehensive risk assessment, land configuration studies or other activities that are pertinent to Site closure. Activities that are outside of the direct control of the AME group may not follow this document even though the data generated from those activities may be used in supporting Site closure.

Data from the non-controlled activities that support Site closure will be assessed on an individual basis. The pathways that are covered in this document include

- Runoff / Diffuse Overland Flow
- Surface Water Flow
- Groundwater Transport - both saturated and unsaturated
- Erosional Transport
- Airborne Transport

For this document, the DQO process focuses on the overriding goal of the Rocky Flats Cleanup Agreement (RFCA) and AME goal to protect surface water. Investigation of the airborne transport pathway is equally important, and study of the air pathway was initiated in FY99 and will be completed in FY00. DQOs for investigation of airborne actinide transport have been incorporated into this document.

## **DATA QUALITY OBJECTIVES**

### **The Problem**

The actinide migration studies are designed to determine what actinide concentration level in environmental media are likely to cause exceedances in surface water or air quality standards at or beyond the formal Site boundaries (currently the Site fenceline).

### **The Decision**

- 1) Are the collective inputs and outputs of the model(s) within acceptable uncertainties to venture further decisions that depend upon the AME outcome, e.g., acceptable risk to human health, exceedance of action levels, or whether to remediate?
- 2) Does the current concentration of actinides in environmental media cause exceedances of the surface water quality standards and/or air quality standards in given future scenarios?

### **Inputs to the Decision**

The inputs to the decision will be the results of many modeling events (see Table 1) and analytical measurements. The modeling results combined with analytical data will be evaluated to determine unique conditions and media-specific concentrations that may likely cause exceedances of surface water or air quality standards. The data inputs for the models are identified in Table 2 (Potential Model Needs).

Data from the non-controlled activities that support Site closure will be assessed on an individual basis. The pathways that are covered in this document include

- Runoff / Diffuse Overland Flow
- Surface Water Flow
- Groundwater Transport - both saturated and unsaturated
- Erosional Transport
- Airborne Transport

For this document, the DQO process focuses on the overriding goal of the Rocky Flats Cleanup Agreement (RFCA) and AME goal to protect surface water. Investigation of the airborne transport pathway is equally important, and study of the air pathway was initiated in FY99 and will be completed in FY00. DQOs for investigation of airborne actinide transport have been incorporated into this document.

## **DATA QUALITY OBJECTIVES**

### **The Problem**

The actinide migration studies are designed to determine what actinide concentration level in environmental media are likely to cause exceedances in surface water or air quality standards at or beyond the formal Site boundaries (currently the Site fenceline).

### **The Decision**

- 1) Are the collective inputs and outputs of the model(s) within acceptable uncertainties to venture further decisions that depend upon the AME outcome, e.g., acceptable risk to human health, exceedance of action levels, or whether to remediate?
- 2) Does the current concentration of actinides in environmental media cause exceedances of the surface water quality standards and/or air quality standards in given future scenarios?

### **Inputs to the Decision**

The inputs to the decision will be the results of many modeling events (see Table 1) and analytical measurements. The modeling results combined with analytical data will be evaluated to determine unique conditions and media-specific concentrations that may likely cause exceedances of surface water or air quality standards. The data inputs for the models are identified in Table 2 (Potential Model Needs).

*Table 1-Summary of basic actinide transport processes and associated actinide sources and models to be assessed.*

<b>Actinide Migration Pathway</b>	<b>Examples of Model Types To Be Assessed</b>	<b>Transport Process</b>	<b>Actinide Source Media</b>
<b>Runoff / Diffuse Overland Flow</b>	WEPP Water Erosion Prediction Project	Sediment/Particulate Transport by Overland Flow	Soil & Sediment (note sediment includes vegetation fragments)
<b>Surface Water Flow</b>	HEC-6T Sediment Transport in Stream Networks	Sediment / Particulate Transport in Stream Water Flow and Catchment Deposition	Erosion from Surface Soils, Channel Bottom Sediment Resuspension
<b>Groundwater Flow (Unsaturated and Saturated)</b>	Geochemical Model W/ATEQ4F and FREQ	Dissolution, Speciation, Precipitation, Colloidal/Particulate Transport by Macropore Flow	Surficial Contamination, Buried Wastes (e.g. Trenches), Buried Utilities, Process Waste Lines, Under Building Contamination
<b>Airborne Transport</b>	Industrial Source Complex 3 Multiple Source Gaussian Plume	Resuspension Particulate Transport	Site Emissions, Contaminated Soils, D&D of Facilities

#### Urgent Data Needs for Decision Input

Table 2 provides an outline of the transport processes, models, and associated source media for predictive modeling of actinide mobility at the Site. The table lists new and existing data that will be needed to determine the causes of current surface-water quality standard exceedences in Walnut Creek. The evaluation (quality assessment) of the input data used for the models and/or specific analytical criteria are discussed later in this document.

#### Near and Long-Term Data Needs for Decision Input

The AME modeling will address pre-closure and post-closure phases of Site operation for both normal and extreme conditions (e.g., 100-year precipitation event). In the near-term, remediation efforts and decommissioning of the Site might cause changes in actinide mobility. Similarly, after Site closure, there will remain a residual level of contamination, which will be managed or controlled sufficiently to protect surface-water and other natural resources. Therefore, the data needs for modeling the near-term and long-term effects of actinide migration on surface-water and air quality are more extensive than the urgent data needs for determining the cause of current water-quality impacts to Walnut Creek. The following table presents the data needs, availability, and attainability for study of near-term and long-term effects. The evaluation (quality assessment) of the input data used for the models and/or specific analytical criteria are discussed later in this document.



**Table 2 — Data needs, availability, and attainability for investigation of water-quality standard exceedances**

Actinide Migration Pathways / Processes	Potential Model Needs	RFETS Data Availability	Description of Existing / New Data Attainability	Limits on Data Uncertainty
Diffuse Overland Flow / Soil Erosion	Soil Particle Size	Data are available from Site Databases and CSM and TAMU Research for AME and USEPA	Site Data from OU Soil Properties CSM Particle Size Distribution of Pu and Am for 12 Soil Samples and 3 Sediment Samples TAMU Particle Size Distribution of Pu and Am in Site Surface Water at GS10 and GS03	Data Quality is Consistent with PARCC Parameters Herein Data are Suitable for Site Reports or Refereed Journals
	Actinide Distribution by Particle Size Soil Properties Soil Isotopic Activity/ Spatial Distribution	Samples from more than 2000 Locations were Suitable for Spatial Analysis (Kriging)	OU Investigations, Research in OU2, 903 Characterization, AME Sampling, Surface Water Source Evaluation Sampling	All Data Will Be Consistent With PARCC Parameters Described in this Document
	Suspended Solids Concentrations Suspended and Bed Material Grain Size Distributions, Sediment Depth and Activities	Limited Surface Water Data are Available AME Data from SID and HEC-6T Field Investigations in 1999 are Available	Data are Available for Selected Gaging Stations for Storm Runoff Events Bed Material Grain Size Estimated in 1999 Survey for HEC-6T Model Input Sediment Depth Estimates for the SID from AME Site Pond Data from OU5 and 6 RI/RFIs	Distribution Should Include Size Range from 2 mm to 2 $\mu$ m Data are Needed for the Percentage of Material in Each WEPP- and HEC-6T-Specified Size Fractions Detection Limit = 1 mg/L Sediment Depth Estimates to +/- 1 Inch All Analytical Data Will Be Consistent With PARCC Parameters Described in this Document
	Surface Water Isotopic Activity	Available	7-Year Surface Water Record Available, Length of Record Varies by Sampling Station	All Data Will Be Consistent With PARCC Parameters Described in this Document
	Stream Discharge	Available	7-Year Record Available, Length of Record Varies by Sampling Station	0 1 Cubic Feet Per Second
	Sediment Load, Isotopic Activity	Limited Data Available	5-Year Surface Water Record Available, Length of Record Varies by Sampling Station	All Data Will Be Consistent With PARCC Parameters Described in this Document
	Sediment Sources / Sinks	Mapping Available GIS Coverage's also Available Sampling Planned for FY00	Attainable from Mapping, GIS Analysis, Field Inspection, Observations, and Sampling	2-Foot Contour Mapping, Visual Observation Sediment Sampling Depth to +/- 1 inch

Actinide Migration Pathways / Processes	Potential Model Needs	RFETS Data Availability	Description of Existing / New Data Attainability	Limits on Data Uncertainty
	Landscape Slope values, Hill slope Dimensions	Available	2' and 5' GIS Contour Mapping	2-foot Contour Interval Resolution
	Channel Geometry	Available	Contained in Site Master Plan and 1999 Field Survey for HEC-6T Model	2-foot Contour Interval Resolution on Mapping 0.5 Foot Resolution for Field Survey
	Catchment Characteristics	Available	Contained in Pond Operations Model, Dam Inspection Reports from SEO	2-Foot Contour Interval Resolution
	Climate / Precipitation	Available	RMRS Surface Water has all Available Historic Precipitation Complete Climate Data Available for 1995-98	Precip = 0.01 Inch Resolution on 15-Minute Increments, Temp = 1°C per 15 Minutes, Wind = 1 mph per 15 Minutes
	Vegetation Canopy, Cover, & Type, Growth Characteristics	Available	Vegetation Maps Prepared, Ecological Monitoring Reports, EMSP Rainfall Simulator Study Data (CSU) Two Years Monitoring of 12 Habitats used for Erosion Model Input and Calibration	Vegetation and Cover are Highly Variable and an Average Value will be Used
	Rill / Inter-Rill Characteristics	Available	Field Observations and Data Recorded at 50 Locations from 1998 for Surface Water Source Evaluation Soil Sampling and Site Vegetation Survey	Uncertainty Estimated to be as High as +/- 40%
	Soil characteristics	Available	Soil Type, Texture, Bulk Density, Hydraulic Conductivity, Organic Content, Depth, Cover, Roughness from Site Data	High Degree of Spatial Variability for all Soil Parameters
	Calibration Data	Available	EMSP Rainfall Simulator Study Data (CSU)	Replicates were Performed and Variability Among Plots will be Determined
Phase Association Affect on Mobility in Surface Water and Groundwater	Actinide Oxidation State, Oxidation/Reduction Effects, & Phase Association (Kd)	EMSP/ AME Research	CSM Research Concluded in 1999 Addressed Kd and Redox Affects on Pu and Am Continuing USEPA Research at CSM Addresses Soil Association LANL Work in 1999 Determined Pu/V Oxidation State	Consistent with PARC Parameters Identified Herein

Actinide Migration Pathway / Process	Potential Model Needs	RFETS Data Availability	(PuO <sub>2</sub> ) under 903 Pad Description of Existing / New Data Attainability	Limits on Data Uncertainty
	Factors Affecting Dissolution and Transport (e.g. pH, Eh, TOC, DOC, Colloids, Others)	AME Research	Research by TAMU in FY99/FY00 Addresses Mechanisms of Aqueous, Suspended Transport	All Data Will Be Consistent With PARCC Parameters Described in this Document
Groundwater Transport - Including Unsaturated Flow	Near-Surface and Subsurface Isotopic Activity	Available but May be Limited in Some Areas	Surface Soil Data in RFEDS and SWD	All Data Will Be Consistent With PARCC Parameters Described in this Document
	Vertical Distribution of Activity	Available for OU2, Limited Elsewhere	RFEDS / SWD	All Data Will Be Consistent With PARCC Parameters Described in this Document
	Factors Affecting Dissolution in Groundwater/Interflow	In Progress/USGS	OU2 Research EMSP & AMS Research	Varies, Based on individual Work Plan
	Actinide Oxidation State	CSM FY99 Research, Others in Progress	OU2 Research EMSP & AMS Research Research	Varies, Based on individual Work Plan
	Subsurface Particle Mobility	Some Information Available	USGS Research, OU2 Research	1 meter +/-year
	Hydro-strat Unit and Soil Composition Mineralogy, Organic Content	Available	Well Drilling Programs General Mineralogy	Varies, Based on individual Work Plan All Analytical Data Will Be Consistent With PARCC Parameters Described in this Document

FY2000 Actinide Migration Evaluation  
Data Quality Objectives  
April 11, 2000, FINAL Revision 6

Actinide Migration Pathway / Process	Potential Model Needs	RFETS Data Availability	Description of Existing / New Data Attainability	Limits on Data Uncertainty
	General Water Quality pH, Eh (by FeII/FeIII or D O ), Conductivity, Temperature, TOC/DOC	Minimal Amount of Data for Eh No Data for FeII/FeIII All others available from Site Monitoring	Could Implement eh Monitoring at Selected Wells, Records of Eh and Other Parameters Varies by Well, 1991-Present	pH 0.1 unit Eh 0.1 millivolt Conductivity 100 µS/cm Temp 1 °C TOC/DOC 0.1 mg/L
	Potential Complexing Species	In Progress	OU2 Research EMSP, AME, and USGS Research	90% Confidence in Accurate Identification of Complexing Species
	Water Balance	Several Completed to Date but New Study Began in FY00	SWD Conducted Site-wide Water Balance for IA IM/IRA, Pond Operations, and Other Projects Current Site Wide Water Balance Project is Underway	+/- 500,000 gallons / year
Interflow (Near Surface Saturated Flow) / Particulate and Solute Transport	Interflow Properties e.g. Precipitation Required, Areas Where Important Soil Properties, Subsurface Geology, Define from Saturated Flow	Some Areas Identified, But Others Need To Be Identified	Data Should be Available from RI/RFI Reports Hydrologic Data are Available in some Areas	Need to Know Areas, Depth to Water Table and to Interflow Zone +/- 10%, Depth to Bedrock +/-10%, Conductivity Measurements are Highly Variable
	Near-Surface and Subsurface Isotopic Activity	Available May be Limited in Some Areas	Surface Soil Data in RFEDS and SWD	All Data Will Be Consistent With PARCC Parameters Described in this Document
	Vertical Distribution of Activity	Available in OU2, Limited Elsewhere	RFEDS / SWD	All Data Will Be Consistent With PARCC Parameters Described in this Document
	Factors Affecting Dissolution in Groundwater/Interflow, Hydrologic Properties	In Progress	OU2 Research EMSP & AME Research	All Data Will Be Consistent With PARCC Parameters Described in this Document

12

Actinide Migration Pathways / Processes	Potential Model Needs	RFETS Data Availability	Description of Existing/New Data Attainability	Limits on Data Uncertainty
Airborne Transport	Meteorological Data	Data Available	Site Meteorological Monitoring Data from 61 m Tower Nearby Meteorological Monitoring Data is Also Available from CDPHE	Wind Speed = +/- 0.2 m/s + 5% of Observed Wind Direction = +/- 5.0 deg Temp = +/- 0.5 deg C
	Topography	Data Available	Data Available from USGS	2 Foot Contours
	Emissions Data	Data Available	On-Site and OU-3 Wind Tunnel Studies/Monitoring	All Data Will Be Consistent With PARCC Parameters Described in this Document
	Particle Size Data	Data Available	On-Site Monitoring Data <sup>a</sup>	1 µm
	Isotopic Distribution Among Particle Sizes	Data Available	On-Site Monitoring Data <sup>a</sup>	All Data Will Be Consistent With PARCC Parameters Described in this Document
	Ambient Isotopic Data	Data Available	On-Site Monitoring Data from Site and CDPHE	Minimum detection limit of 0.1 mrem
	Surface Soil Actinide Spatial Distribution	Data Available	Site Soil Spatial Analysis (Kriging) (2000 Measurements)	All Data Will Be Consistent With PARCC Parameters Described in this Document Additionally, Geostatistics Variance may be Mapped for Error Analysis

Notes

<sup>a</sup>Reference Langer, G , 1987 *Dust Transport—Wind Blown and Mechanical Resuspension* HS&E Applications Technology Semiannual Progress Report May

Data needs shown in the previous Tables will be specifically designated within the individual work plans and the Tables will be refined as the actinide migration processes and pathways are better understood. Additionally, the limits on data uncertainty are current best estimates and the actual limits will be described in the individual work plans and activity results.

### **Study Boundaries**

Investigation of actinide migration processes will be conducted on a Site (and nearby off-Site areas) watershed basis with respect to surface water quality. Airborne transport studies will concentrate on the immediate Site and nearby off-Site areas. However, the study boundaries will be altered to be consistent with changes in facilities and the environment per the Site Vision to address urgent, near-term, and long-term protection of surface water quality and air quality. Any changes in the general model boundaries stated, especially extrapolation of predictions beyond these 3-dimensional and temporal boundaries, shall be explicitly addressed in associated reports of model results.

#### Boundaries for Urgent Protection of Surface Water

The geographic boundaries for the AME are the watershed boundaries for the Walnut Creek watershed. The study is also bounded by the limits of current understanding of actinide chemistry and environmental mobility.

#### Boundaries for Near-Term Protection of Surface Water

The geographic boundaries for the AME are the watershed boundaries for the South Interceptor Ditch drainage, Woman Creek and the Walnut Creek watersheds. These drainage basins will have the potential for contributing to SW degradation during remediation activities. The study is also bounded by the limits of current understanding of actinide chemistry and environmental mobility.

#### Boundaries for Long-Term Protection of Surface Water

The geographic boundaries for the AME are the watershed and associated airshed boundaries for the Woman Creek and Walnut Creek watersheds. This study area would be affected by the elimination of the industrial area and elimination or reconfiguration of the detention pond systems and possible filling of the interceptor ditch structures. The study is also bounded by the limits of current understanding of actinide chemistry and environmental mobility.

#### Boundaries for Near and Long-Term Protection of Air Quality

The geographic boundaries for near-term airborne transport are the Site and nearby areas within a kilometer of the Site fenceline in the predominant wind direction. For long-term transport, additional areas to the east of the Site (downwind) will be included.

## **Decision Rules**

- 1) If uncertainties are clearly defined for model inputs and outputs and the uncertainties are considered reasonable within the related scientific/engineering framework (based on multiple levels of peer review by all applicable disciplines), then AME results may be used in the next step of decision-making (relative to actinide impacts on human health and the environment) Otherwise, uncertainties within the AME are too great to make informed decisions without further model (input and/or output) refinement
- 2) If results of the analytical data and modeling efforts indicate that current action levels or remediation techniques are inadequate to be protective of surface water and/or air quality standards, then action levels will be revised or additional actions will be defined to limit or prevent surface water or air quality exceedances and to enhance protection of long-term downstream uses Otherwise, the current (actinide) status quo does not present significant risk to surface water and/or air quality standards

NOTE Any action level changes or additional remedial actions that are proposed will be based on the integration of all analytical and modeling activities conducted under the AME group, as well as data generated by other entities outside of the AME group

## **Limits on Decision Errors**

De facto error limits do not exist for modeling purposes within the AME context, but there is, rather, a necessity to quantify errors resulting from the model(s) to maintain perspective when model results are considered for high level policy decisions -- e g , land use or whether to remediate In particular, error ranges must be explicitly defined for all inputs, output errors must be clearly related to model calibration results and sensitivity analyses Error terms will be quantified as the sensitivity of the models and the relevant transport mechanisms are identified and quantified

## **Optimization of Design**

Models, including inputs and/or outputs, will be optimized if associated uncertainties are concluded as unacceptable as per the DQOs

## **Limits of Measurement Uncertainty**

The actinide studies at RFETS are an important component of the overall closure of the Site and will impact action levels and remedial approaches Additionally, these results will undergo intense scrutiny by the Site, stakeholders, and regulatory agencies

Therefore, the acquisition of statistically well-quantified, scientifically defensible data is critical to the successful completion of the closure project

The criteria specified below are general in nature and will be modified as each scope of work is delineated. Specific QA/QC requirements for laboratory procedures and analyses are captured in the K-H Analytical Services Division (ASD) subcontract requirements and site-specific procedures (all accessible on the RFETS intranet). Unique circumstances will be addressed in project-specific controlling documents (for the required analytical and extraction methods, etc.) to support decisions as needed. The criteria for modeling will also be developed on an individual basis, however, the criteria described below are the minimum requirements that must be addressed.

### **Analytical Requirements**

#### **Accuracy**

For standard analytical procedures the following minimum measurements of accuracy will be followed:

- Calibration of the instrument prior to analysis and as specified in the specified methods on a continuing basis
- Laboratory Control Samples will be analyzed at a rate of  $\geq 1/20$  (or per batch, whichever is more frequent)
- Matrix spikes and Matrix Spike Duplicates will be analyzed at a rate of  $1/20$
- Both method and equipment blanks will be analyzed at a rate of  $\geq 1/20$  (or per batch, whichever is more frequent)
- Chemical yields will be calculated
- Counting times will be recorded
- Detector efficiency will be calculated

For unique or experimental analytical procedures accuracy will be addressed through the use of uncertainty calculations (defined in the individual work plans). Uncertainties for all processes conducted will be estimated on the basis of industry accepted statistical practices, unless the uncertainties are truly non-measurable or insignificant to the total propagated uncertainty, in which case they will be discussed but not quantified. All uncertainties will be estimated at the 95% confidence interval.

At a minimum, radioisotope analytical processes utilized for AME projects will set the following limits as expected quality assurance measures for the minimization of data uncertainty.

16



Therefore, the acquisition of statistically well-quantified, scientifically defensible data is critical to the successful completion of the closure project

The criteria specified below are general in nature and will be modified as each scope of work is delineated. Specific QA/QC requirements for laboratory procedures and analyses are captured in the K-H Analytical Services Division (ASD) subcontract requirements and site-specific procedures (all accessible on the RFETS intranet). Unique circumstances will be addressed in project-specific controlling documents (for the required analytical and extraction methods, etc.) to support decisions as needed. The criteria for modeling will also be developed on an individual basis, however, the criteria described below are the minimum requirements that must be addressed.

### **Analytical Requirements**

#### **Accuracy**

For standard analytical procedures the following minimum measurements of accuracy will be followed:

- Calibration of the instrument prior to analysis and as specified in the specified methods on a continuing basis
- Laboratory Control Samples will be analyzed at a rate of  $\geq 1/20$  (or per batch, whichever is more frequent)
- Matrix spikes and Matrix Spike Duplicates will be analyzed at a rate of  $1/20$
- Both method and equipment blanks will be analyzed at a rate of  $\geq 1/20$  (or per batch, whichever is more frequent)
- Chemical yields will be calculated
- Counting times will be recorded
- Detector efficiency will be calculated

For unique or experimental analytical procedures accuracy will be addressed through the use of uncertainty calculations (defined in the individual work plans). Uncertainties for all processes conducted will be estimated on the basis of industry accepted statistical practices, unless the uncertainties are truly non-measurable or insignificant to the total propagated uncertainty, in which case they will be discussed but not quantified. All uncertainties will be estimated at the 95% confidence interval.

At a minimum, radioisotope analytical processes utilized for AME projects will set the following limits as expected quality assurance measures for the minimization of data uncertainty.

- Alpha spectrometer will be energy calibrated over the range of analytes and tracers anticipated by the study (approx 4-7 MeV) Calibration verifications will be performed on a weekly basis Recalibration will be performed when any of the peaks across the spectrum are not within 40 keV of the expected energy
- Efficiency calibration will be performed once at the beginning of the project and used to calculate chemical yields only Internal tracers will provide the efficiency information necessary to calculate the activities of the analytes
- < 75% tracer recovery will prompt an evaluation of the data for meeting the data quality objectives If the uncertainty criteria are met, no further action will be taken If not, a reanalysis will be performed unless circumstances prevent a reanalysis (e g , limited sample mass) <30% tracer recovery will be considered limited use data with possible reanalysis depending on the impact on the project <10% tracer recovery will prompt reanalysis and/or data considered unusable In both of the latter cases, reanalysis will be the first choice for corrective action Other actions may be taken depending on the impact to the study
- Analytical parameters will be set to achieve sample specific MDAs less than or equal to 0.3 pCi/gram, unless sample exceeds 10 times the MDA (as calculated in RFETS SOW - Alpha Spectrometry Module) Counting times will be recorded as a part of this function
- Parameters will be used to achieve 2 sigma (95%confidence interval) analytical propagated uncertainties (not including sample variability) of less than 20% where the activity of the fraction exceeds 0.3 pCi/g Count times will be at least 1000 minutes, in order to achieve the lowest reasonable counting uncertainty, if the 2 sigma (95%confidence interval) counting uncertainty exceeds 5% otherwise
- Matrix spikes will be performed on no less than 1 in 20 of the selective extraction samples An assessment of the overall recovery of the spike from all of the fractions will be reported Qualified interpretation of these results will be documented in the final report
- Laboratory Control Samples (LCS) will be analyzed on a frequency of 1 in 20 An LCS will be a blank matrix spiked with the analyte(s) of interest
- Blanks (using quartz sand as a matrix) will be performed at no less than 1 in 20 samples or with every batch whichever is more frequent
- Sample variability will be determined through radioanalytical and statistical means which will then be used to propagate the total uncertainty based on all processes performed at CSM The calculations for obtaining these uncertainty data will be documented and reported
- All standard solutions will be Standard Reference Materials from NIST or calibrated standards from a vendor that is traceable to NIST

## Precision

At a minimum, the following measurements of precision will be used for all analytical processes, unless otherwise specified in the individual approved work plan

- Duplicate error ratio (DER) will be calculated as a measure of precision for radionuclide analysis and the relative percent difference (RPD) will be calculated for all other measurements unless a satisfactory alternative is specified in the approved work plan
- Measurement precision will be addressed by analyzing replicate samples of no less than 1:20 as duplicates. Replication will exceed this minimum when it is determined that the variability of the process may introduce more than 10% of the total propagated uncertainty. For example, it is hypothesized that the variability in the sub-sampling of field samples may be introducing more than 10% of the total propagated uncertainty of the Pu-239/240 contamination found in the various fractions of the selective extraction analytical process. Therefore, in order to estimate this contribution of uncertainty, at least three replicates of varying quantities of dried, mixed soil (not pulverized due to the disturbance of the natural binding properties) will be analyzed for optimizing the aliquot size to achieve the lowest reasonable uncertainty. The variability will be used as an estimate of the sub-sampling uncertainty and propagated with the other analytical uncertainties.
- Field duplicates will be analyzed for all analytical procedures as described in the work plan or at a minimum rate of 1:20, and will be submitted blind to the analytical lab.

### **Representativeness**

- Chains-of-custody will be properly completed and signed
- Work plans will be approved by the Site and followed

### **Comparability**

- Established analytical methods will be used
- All analytical/radiochemistry protocols will be documented and/or referenced
- SOPs will be written and further documentation produced of sufficient detail that the experimentation could be reproduced at an independent laboratory of equivalent technical capability. Documentation will generally follow the guidelines as set forth in RFETS SOW - GENERAL LABORATORY REQUIREMENTS, MODULE GR01 B1 where applicable to the nature of this experimental work and as reasonable within the scope of the individual project.

## **Completeness**

- The number of samples analyzed ( both real and QC) will match the work plan

## **Statistical Sampling/Sub-Sampling**

A statistical basis for the sample collection (and sub-sampling) will need to be developed on a case-by-case basis in accordance with EPA guidance or other established references DQOs must be established for each unique decision set and population from which the samples are taken

## **Validation**

All analytical data will be validated at a minimum of 25% by an independent third party consistent with Site standards Laboratories will be audited on a periodic basis

## **Model Requirements**

Models must comply with minimal DOE QA requirements as defined in DOE Order 414 1, Quality Assurance, Section 4 b (2)(b) and (2)(d) The former requirement calls for “sound engineering/scientific principles”, “incorporation of design bases”, and “verification or validation by individuals other than those who performed the work” The latter requires “ testing of processes using established acceptance and performance criteria” To accomplish these ends, implementation of these requirements must explicitly communicate *how* each model is scientifically/technically sound (defensible), what the specific design bases consist of, and finally, what the acceptance and performance criteria consist of prior to actual use of the model(s)

Further, implementation of the requirement, as described in the following subsections, will allow verification and validation of the models by independent reviewers The processes of determining model sensitivities and uncertainties and calibration of the model shall be documented Verification and validation by independent reviewers will be facilitated proportional to the quality of said documentation

## **Sensitivity and Uncertainty Analysis**

The process of model sensitivity and uncertainty analysis is best described as an analysis that encompasses all of the parameters (inputs and outputs), tabulated functions, and driving variables in the model The requirements specified in this section are of a broad

nature to help encompass the variety of models that will be utilized to support the AME activities. Any unique sensitivity and uncertainty modeling requirements that may not be addressed in this section should be described in the individual work plans. Additionally, any component that is either not applicable or unachievable should be described in the work plan. The implied requirements for AME model sensitivity and uncertainty analysis are as follows:

- All input and output data shall be defined, all values will be adequately labeled and explained, including engineering units for each variable
- All assumptions associated with the model, together with the pertinent rationale supporting those assumptions, shall be defined
- A sensitivity analysis shall include verification that qualitative behavior of the model output conforms to expectations
- A logical sensitivity analysis should be performed to identify inputs for which an output is entirely insensitive (factor screening). These screening inputs may then be ignored in subsequent analyses if the sensitivity of said input is independent of all other model inputs
- Sensitivity of the model to each influential input parameter must be described in terms of how it affects, or influences, the model's output; this sensitivity is usually described as a specific range in the output's value relative to a corresponding range in the input's value, while all other inputs are held constant
- Significant interaction between inputs shall be documented
- Whenever possible, define the uncertainty for each input parameter. Information about data correlation in uncertain inputs can be quite valuable since such information may greatly reduce output uncertainty
- Estimate the total propagated uncertainty associated with each model output, which includes and discusses use of stated input uncertainties. Probabilities associated with each uncertainty may also be useful in narrowing a range of values to the most likely point-value (given confidence expectations of the regulators, the public, or the customer)
- If artificially generated weather data are used, the weather-generating model should also convey similar V&V checks whenever possible

21

nature to help encompass the variety of models that will be utilized to support the AME activities. Any unique sensitivity and uncertainty modeling requirements that may not be addressed in this section should be described in the individual work plans. Additionally, any component that is either not applicable or unachievable should be described in the work plan. The implied requirements for AME model sensitivity and uncertainty analysis are as follows:

- All input and output data shall be defined, all values will be adequately labeled and explained, including engineering units for each variable
- All assumptions associated with the model, together with the pertinent rationale supporting those assumptions, shall be defined
- A sensitivity analysis shall include verification that qualitative behavior of the model output conforms to expectations
- A logical sensitivity analysis should be performed to identify inputs for which an output is entirely insensitive (factor screening). These sleeping inputs may then be ignored in subsequent analyses if the sensitivity of said input is independent of all other model inputs
- Sensitivity of the model to each influential input parameter must be described in terms of how it affects, or influences, the model's output; this sensitivity is usually described as a specific range in the output's value relative to a corresponding range in the input's value, while all other inputs are held constant
- Significant interaction between inputs shall be documented
- Whenever possible, define the uncertainty for each input parameter. Information about data correlation in uncertain inputs can be quite valuable since such information may greatly reduce output uncertainty
- Estimate the total propagated uncertainty associated with each model output, which includes and discusses use of stated input uncertainties. Probabilities associated with each uncertainty may also be useful in narrowing a range of values to the most likely point-value (given confidence expectations of the regulators, the public, or the customer)
- If artificially generated weather data are used, the weather-generating model should also convey similar V&V checks whenever possible

- Simple random sampling (or other statistically viable techniques) is recommended to determine and document the input uncertainty distribution
- Parameters should be ranked as to their contribution to output uncertainty
- Parameters should be ranked as to their sensitivity (on model output)

### **Calibration**

The process of model calibration is best described as an adjustment of the model such that model output matches “real-world” behavior. It should be noted the requirements specified in this section are of a broad nature to help encompass the variety of models that will be utilized to support the AME activities. Any unique modeling calibration requirements that may not be addressed in this section should be described in the individual work plans. Additionally, any component that is either not applicable or unachievable should be described in the work plan. The implied requirements for AME model calibration are as follows:

- The calibration method must not result in the generation of a physically impossible parameter vector (output)
- Input parameters of the model must be consistent with measured values or values within the expected parameter ranges of the system being modeled
- A clear comparison between predicted values (model output) and measured values of the modeled phenomenon of interest
- The calibration method to be chosen should use the results from a one-at-a-time parameter sensitivity analysis to determine whether the implicitly defined relations between state variables and parameters are continuous or discontinuous and linear or nonlinear. If the model response is smooth, the model can be linearized, and a fast optimization procedure using a locally linear approximation may be possible. If the response is discontinuous, a more robust calibration procedure should be used.
- During the calibration process, parameter probability values, based on literature reviews or on well-documented expert knowledge, should be assigned if possible
- If the model is not embedded in a parameter estimating procedure, calibration should be executed as follows: Use sensitivity analysis to analyze relations between state variables. Determine independent subsystems, and calibrate the individual subsystems, taking care that once a subsystem is calibrated, that subsystem is not

modified in following calibration steps

- When possible, estimate input parameters simultaneously
- The uncertainty of the parameters after calibration should be derived under the following conditions The model is correct and the non-calibrated parameters have a negligible effect on the output uncertainty To investigate the effect of non-calibrated parameters an uncertainty analysis should be performed
- If a model (estimate) for the measurement error is available, and the calibration criteria is based on it, then a set- or distribution calibration may be conducted Both calibrations allow quantification of the total uncertainty about crucial model outputs after calibration This uncertainty should be reviewed and deemed acceptable for the specific application
- All calibration criteria will be adequately described and documented

### **Model Verification/Validation**

The process of model V&V (the assessment of model adequacy) consists of a robust review of the model's documentation and utility V&V includes assessing all aspects of the model's assumptions, inputs, outputs, sensitivities, and uncertainty, with particular emphasis on calibration results and limitations (comparison of the models output to a corresponding measured value(s)) V&V incorporates quality requirements arising from DOE Order 414 1 Section 4 b, as well as other applicable guidance or standards applicable to the natural phenomenon or numerical model of interest

Verification activities include the inspection of the internal consistency of the model and its software implementation Some important elements are 1) analysis of dimensions and units, 2) on-line checks on mass conservation, and 3) detection of violation of natural ranges of parameters and variables Verification also comprises inspection of qualitative behavior of the model and its implementation, for instance, checks as to whether the response of model output, relative to systematic changes in values of input parameters, conforms to theoretical insights

Model validation includes establishing the usefulness and relevance of a model for a predefined purpose Models have always a limited range of validity, and it is necessary to define the useful range (and thus limitations) of the model In case of predictive models, a major part of the validation consists in assessing prediction accuracy

The requirements specified in this section are of a broad nature to help encompass the



variety of models that will be utilized to support the AME activities. Any unique modeling V&V requirements that may not be addressed in this section should be described in the individual work plans. Additionally, any V&V component that is either not applicable or unachievable should be described in the work plan. The implied requirements for AME model verification/validation process are as follows:

- Explicitly define for what purpose the model is being used, and compare this with the objectives for which the model was developed
- Define and describe any limitations on the model (e.g., physical/chemical processes, assumptions, or natural phenomenon that would render model output as not applicable)
- A key component of model validation is to show the model is of practical use for a specific purpose over a specified range. Additionally, a discussion of acceptable error size, with due regard to the specific purpose, should be included. Large errors might make the model of little practical value as a predictor, though it might still have an instructive value.
- Software quality elements, especially calibration of the original computer code (inputs to outputs) and clear traceability (documentation) of any modifications/revisions to the original code
- If the model is to be used in predictions, such as scenario studies, the validation of the model will focus on parameters of interest that could influence differences between scenarios, or the resulting ranking of alternatives
- The validation data should be representative for the situations in which the model is to be used. The validation set should cover the range of situations encountered in predictions
- The calibration data and the validation data should be different, if possible
- Model validation must be repeatable by peers. All validation data (in a broad sense, comprising input, output, and model structure) shall be documented and accessible for independent review
- Reproducible model calibrations should be presented
- A sensitivity analysis of the model that includes systematic variations to the inputs relative to the model output should be documented

- If the subject of a model (area, etc ) is too large for a standard validation approach (e g an entire region), the model should be subdivided into components that can be validated separately. If this approach is utilized then provide logical reasoning why the aggregate model is consistent, and identify crucial interactions among the components

## References

(ASCE, 1993) ASCE task force on the Criteria for Evaluation of Watershed Models, Journal of Irrigation and Drainage Engineering, Vol 119, No 3, May/June 1993

(CAMASE, 1995) CAMASE-Guidelines for Modeling, CAMASE News, Newsletter of Agro-ecosystems Modeling, extra edition, November, 1995

USDOE, 1998 DOE Order 414 1, *Quality Assurance*

USEPA, 1994 EPA QA/G-4, *Guidance for the Data Quality Objective Process*

USEPA, 1998 EPA QA/G-9, *Guidance for the Data Quality Assessment Process Practical Methods for Data Analysis*

USEPA, 1999, EPA QA/G-8, *Guidance on Environmental Data Verification and Validation*

26/26